structural bioinformatics - assignment 03 01.12.21

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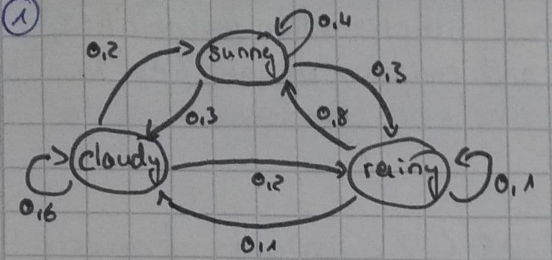


transition probability matrix:

$$A = \begin{array}{c} \\ \text{sunny} \\ \text{cloudy} \\ \text{rainy} \end{array} \begin{array}{c} \begin{array}{ccc} \text{sunny} & \text{cloudy} & \text{rainy} \end{array} \\ \begin{pmatrix} 0{,}4 & 0{,}2 & 0{,}8 \\ 0{,}3 & 0{,}6 & 0{,}1 \\ 0{,}3 & 0{,}2 & 0{,}1 \end{pmatrix} \end{array}$$

We discussed a lot about this exercise and found two ways to interprete it:

1) We want to know the probability, that the weather on the 5th day from today is sunny, given that the other 4 days followed the given path and that today is sunny.

today = sunny path = rainy, rainy, cloudy, sunny, sunny

Since we are looking at a markov model, the weather at day i only depends on the weather at day i-1.
we can calculate the probability as follows

$$p = p(\text{rainy} \mid \text{sunny}) \cdot p(\text{rainy} \mid \text{rainy}) \cdot p(\text{cloudy} \mid \text{rainy}) \cdot p(\text{sunny} \mid \text{cloudy}) \cdot p(\text{sunny} \mid \text{sunny})$$
$$= 0{,}3 \cdot 0{,}1 \cdot 0{,}1 \cdot 0{,}2 \cdot 0{,}4$$
$$= 0{,}00024$$

2) We want to know the probability that the weather on day x is y, only depending on the fact, that today is sunny.

$X_s^{(k)}$ = probability, that it will be sunny k days from now on, no matter what happened in the time in between

$$x^{(k+1)} = A\,x^{(k)}, \quad x^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

day	0	1	2	3	4	5
weather	s	r	r	c	s	s
	$\begin{pmatrix} \boxed{1} \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0{,}4 \\ 0{,}3 \\ \boxed{0{,}3} \end{pmatrix}$	$\begin{pmatrix} 0{,}46 \\ 0{,}33 \\ \boxed{0{,}21} \end{pmatrix}$	$\begin{pmatrix} 0{,}418 \\ \boxed{0{,}357} \\ 0{,}225 \end{pmatrix}$	$\begin{pmatrix} \boxed{0{,}4186} \\ 0{,}3621 \\ 0{,}2193 \end{pmatrix}$	$\begin{pmatrix} \boxed{0{,}4153} \\ 0{,}36477 \\ 0{,}21993 \end{pmatrix}$

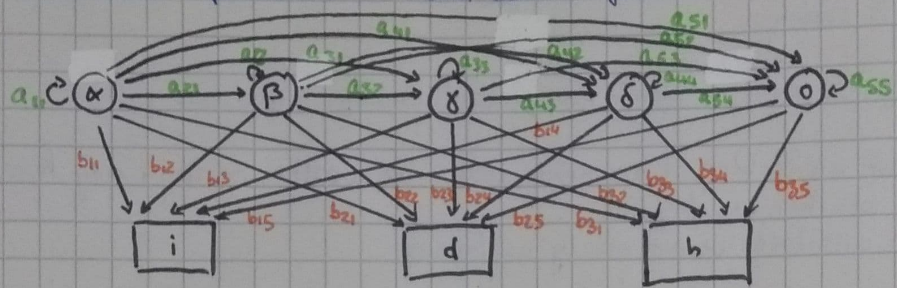
In □ are the probabilities for the different days and the weather on that day labelled.
The probability, that the weather is rainy on the day after tomorrow, given that today is sunny is 0,21.

②

A hidden markov model is a markov process with observable and hidden components.
Every hidden component or state comes with some transmission probabilities, to change into an other hidden state and some emission probabilities, to produce an observable state.

In our example, we thought of using the SARS-CoV 2 variants of concern (as stated by WHO) as hidden states and different rates as infected, deaths or hospitalized as observable states.
To make things a bit easier we assume that mutations can't be created backwards (β can't mutate back to α).

With those informations our model looks as follows:



α = Alpha, B.1.1.7
β = Beta, B.1.351
γ = Gamma, P.1
δ = Delta, B.1.617.2
O = Omikron, B.1.1.529

i = infected / 100.000 residents / 7 days
d = deaths / " "
h = hospitalized / " "

5 hidden states → transition prob. matrix

$$\begin{array}{c|ccccc} & \alpha & \beta & \gamma & \delta & O \\ \hline \alpha & a_{11} & 0 & 0 & 0 & 0 \\ \beta & a_{21} & a_{22} & 0 & 0 & 0 \\ \gamma & a_{31} & a_{32} & a_{33} & 0 & 0 \\ \delta & a_{41} & a_{42} & a_{43} & a_{44} & 0 \\ O & a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{array} = A$$

3 observable states → emission prob. matrix

$$\begin{array}{c|ccccc} & \alpha & \beta & \gamma & \delta & O \\ \hline i & b_{11} & b_{12} & b_{13} & b_{14} & b_{15} \\ d & b_{21} & b_{22} & b_{23} & b_{24} & b_{25} \\ h & b_{31} & b_{32} & b_{33} & b_{34} & b_{35} \end{array} = B$$

③

Sequence logos represent a multiple alignment. Every x position stands for one position in the alignment. The size of the letters matches the relative frequency of the appearence of a certain base at that position.
Since sequence logos represent an alignment, they show which nucleotides are conserved.
Those conserved regions have most of the time a biological meaning, they could be i.e. binding sites of proteins.

Sequence profiles are a set of molecules, i.e. proteins, which are somehow related. Because of that they also have some similar regions.
Sequence profiles are used to decide if a new protein also belongs to the family.

(4)

An artificial neural net mimics a biological brain. The main idea of ANN's is inspired by synapses, which in very simplified terms get some input signal, process it and produce some output signal.
An ANN therefore consists of some input, weights and biases for the processing and generates an output.
Deep neural nets are a subgroup of ANN. To make a neural net "deep" you need more than one hidden layer and a non linear activation function for those layers.